Homology Modeling of the Oxytocin G-Protein Coupling Receptor

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Oxytocin (OT) is a neurohypophysial hormone, which acts both on the peripheral tissues (hormonal), and as a neurotransmitter in the brain. It plays an important role in the control of uterine contractions during labor, secretion of milk and many social and behavioral functions. OT accomplishes its functions via interaction with specific oxytocin receptors, which belong to the rhodopsin-type (class I) group of G-protein coupled receptors (GPCR). High levels of oxytocin during pregnancy are the main cause for preterm birth. Oxytocin receptor antagonists are widely employed for prevention in such cases [1]. Design of these antagonists requires a proper model of the hormone receptor interaction. However, the 3D structure of the OT receptor is not known.

The aim of this investigation is to construct a three-dimensional model of the oxytocin receptor. Protein structure homology modelling is an efficient technique for generating 3D models of proteins in the absence of experimental data. We employed the software package Modeller to generate a family of oxytocin GPCR structures. The assessment of the structures was based on test MD simulations of their interactions with the natural ligand oxytocin.

References

[1] D. Papatsonis, v. Flenady, S. Cole, H. Liley, *Oxytocin receptor antagonists for inhibiting preterm labour (Review)*, 2010 The Cochrane Collaboration. Published by John Wiley & Sons, Ltd.